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=> fil hcaplus
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FILE COVERS 1907 - 24 Dec 2008 VOL 149 ISS 26
FILE LAST UPDATED: 23 Dec 2008 (20081223/ED)
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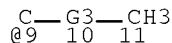
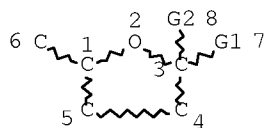
HCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L1 STR
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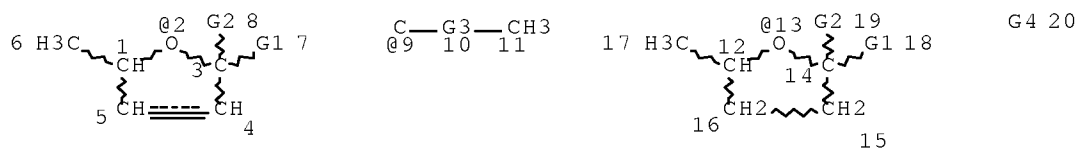


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
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L3 1749 SEA FILE=REGISTRY SSS FUL L1
L4 STR



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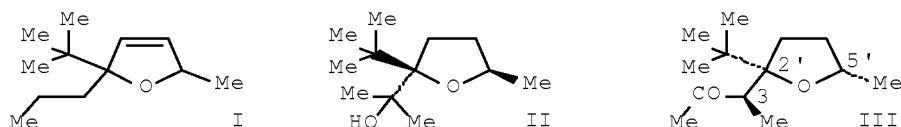
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L10 477297 SEA FILE=HCAPLUS ABB=ON PLU=ON ("ODOR AND ODOROUS SUBSTANCES"
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?ODOR? OR COSMETIC OR SHAMPOO OR DETERGEN? OR PERFUME OR
CLEANER OR LAUNDRY
L11 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 AND L10

=>
=>

=> d ibib abs hitstr l11 1-3

L11 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1174369 HCAPLUS Full-text
DOCUMENT NUMBER: 144:51733
TITLE: Design, synthesis and olfactory properties of
2-substituted 2-tert-butyl-5-methyl-2,5-dihydrofurans:
Seco-derivatives of theaspiranes
AUTHOR(S): Kraft, Philip; Popaj, Kasim; Abate, Agnese
CORPORATE SOURCE: Givaudan Schweiz AG, Fragrance Research, Dubendorf,
8600, Switz.
SOURCE: Synthesis (2005), (16), 2798-2809
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:51733
GI

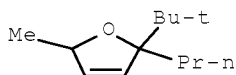


AB Two seco-theaspiranes with pronounced blackcurrant notes, 2-tert-butyl-5-methyl-2-propyl-2,5-dihydrofuran (I) and 2-tert-butyl-5-methyl-2-propyltetrahydrofuran, were synthesized by a synthetic sequence consisting of Grignard reaction, Lindlar hydrogenation, and cyclization followed by optional Pd-catalyzed hydrogenation. The sequence was modified for the synthesis of the oxygenated analogs 2-(2'-tert-butyl-5'-methyltetrahydrofuran-2'-yl)propan-2-ol and 3-(2'-tert-butyl-5'-methyltetrahydrofuran-2'-yl)butan-2-one. The first modification featured trimethylsilyl ether protection and stepwise construction of the alkyne moiety necessitated by steric hindrance. In the second modification, a but-2-en-2-yl group was utilized as latent 3-hydroxybut-1-en-2-yl functionality, and the steric constraint around the tertiary hydroxy group was exploited to introduce a stereocenter by SN2 ring closure. As for the parent compds. 2-tert-butyl-5-methyl-2-propyl-2,5-dihydrofuran and 2-(2'-tert-butyl-5'-methyltetrahydrofuran-2'-yl)propan-2-ol, the odor of the oxygenated seco-theaspiranes was shifted towards a woody tonality. (±)-Trans-2-(2'-tert-butyl-5'-methyltetrahydrofuran-2'-yl)propan-2-ol (II) even had a typical patchouli profile, and (+)-(2'R,3R,5'S)-3-(2'-tert-butyl-5'-methyltetrahydrofuran-2'-yl)butan-2-one (III) and its (-)-(2'S,3S,5'R)-enantiomer differed significantly in their olfactory properties.

IT 871465-49-5P, 2-tert-Butyl-5-methyl-2-propyl-2,5-dihydrofuran
 RL: BSU (Biological study, unclassified); COS (Cosmetic use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (design, synthesis and olfactory properties of 2-substituted 2-tert-butyl-5-methyl-2,5-dihydrofurans, i.e. seco-theaspirane derivs.)

RN 871465-49-5 HCAPLUS

CN Furan, 2-(1,1-dimethylethyl)-2,5-dihydro-5-methyl-2-propyl- (CA INDEX NAME)

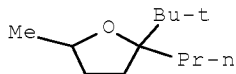


IT 871465-50-8P, 2-tert-Butyl-5-methyl-2-propyltetrahydrofuran
 RL: BSU (Biological study, unclassified); COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(design, synthesis and olfactory properties of 2-substituted 2-tert-butyl-5-methyl-2,5-dihydrofurans, i.e. seco-theaspirane derivs.)

RN 871465-50-8 HCAPLUS

CN Furan, 2-(1,1-dimethylethyl)tetrahydro-5-methyl-2-propyl- (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1021745 HCAPLUS Full-text

DOCUMENT NUMBER: 143:326194

TITLE: Preparation of trisubstituted dihydro- and tetrahydrofurans suitable for use in fragrance compositions

INVENTOR(S): Kraft, Philip

PATENT ASSIGNEE(S): Givaudan S. A., Switz.

SOURCE: PCT Int. Appl., 21 pp.

CODEN: PIXXD2

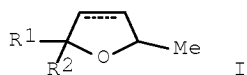
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005087756	A1	20050922	WO 2005-CH137	20050307
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1742929	A1	20070117	EP 2005-706555	20050307
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR			
CN 1930140	A	20070314	CN 2005-80007629	20050307
BR 2005008817	A	20070807	BR 2005-8817	20050307
JP 2007529430	T	20071025	JP 2007-503172	20050307
MX 2006PA10193	A	20061120	MX 2006-PA10193	20060907
KR 2006130214	A	20061218	KR 2006-718843	20060914
IN 2006CN03333	A	20070615	IN 2006-CN3333	20060914
US 20080039360	A1	20080214	US 2007-589654	20070413
PRIORITY APPLN. INFO.:			GB 2004-5723	A 20040315
			WO 2005-CH137	W 20050307
OTHER SOURCE(S):			CASREACT 143:326194; MARPAT 143:326194	
GI				



AB 2,2-Disubstituted 5-methyl-2,5-dihydro- and 2,2-disubstituted 5-methyltetrahydrofurans I (R1 = Me, Et, Pr, Me2CH; R2 = branched C4-7 alkyl, C5-7 cycloalkyl, mono- or disubstituted C5-6 cycloalkyl) are useful as odorants. Thus, treatment of butyn-3-ol with Et Grignard, followed by reaction with 2,2-dimethylhexan-3-one gave 90% 5-tert-butyloct-3-yne-2,5-diol. Hydrogenation in the presence of Lindlar catalyst gave the corresponding (Z)-alkene, which was cyclized by heating in the presence of KHSO4 to give 2-tert-butyl-5-methyl-2-propyl-2,5-dihydrofuran (II). Further hydrogenation of II gave the corresponding THF (III). The odor of II was described as black currant, natural, rich, eucalyptus buds, anise, buchu leaves, slightly green, while III was described as black currant, damascone, sweet, natural, rich, with green, piny, eucalyptus and mint-like facets.

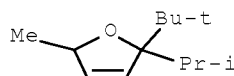
IT ~~865205-21-6P~~ ~~865205-23-8P~~ ~~865205-25-0P~~
~~865205-26-1P~~ ~~871465-49-5P~~

RL: COS (Cosmetic use); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of trisubstituted dihydro- and tetrahydrofurans for use in fragrance comps.)

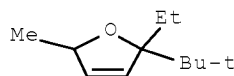
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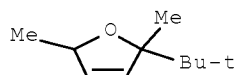
RN 865205-23-8 HCAPLUS

CN Furan, 2-(1,1-dimethylethyl)-2-ethyl-2,5-dihydro-5-methyl- (CA INDEX NAME)



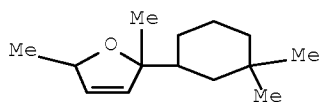
RN 865205-25-0 HCAPLUS

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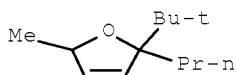


RN 865205-26-1 HCAPLUS

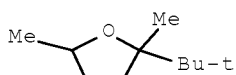
CN Furan, 2-(3,3-dimethylcyclohexyl)-2,5-dihydro-2,5-dimethyl- (CA INDEX NAME)



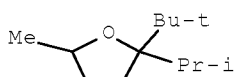
RN 871465-49-5 HCAPLUS
 CN Furan, 2-(1,1-dimethylethyl)-2,5-dihydro-5-methyl-2-propyl- (CA INDEX NAME)



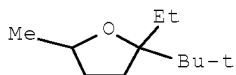
IT 781665-93-8P 865205-22-7P 865205-24-9P
 865205-27-2P 871465-50-8P
 RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of trisubstituted dihydro- and tetrahydrofurans for use in fragrance compns.)
 RN 781665-93-8 HCAPLUS
 CN Furan, 2-(1,1-dimethylethyl)tetrahydro-2,5-dimethyl- (CA INDEX NAME)



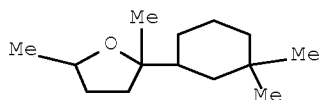
RN 865205-22-7 HCAPLUS
 CN Furan, 2-(1,1-dimethylethyl)tetrahydro-5-methyl-2-(1-methylethyl)- (CA INDEX NAME)



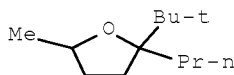
RN 865205-24-9 HCAPLUS
 CN Furan, 2-(1,1-dimethylethyl)-2-ethyltetrahydro-5-methyl- (CA INDEX NAME)



RN 865205-27-2 HCAPLUS
 CN Furan, 2-(3,3-dimethylcyclohexyl)tetrahydro-2,5-dimethyl- (CA INDEX NAME)



RN 871465-50-8 HCAPLUS
 CN Furan, 2-(1,1-dimethylethyl)tetrahydro-5-methyl-2-propyl- (CA INDEX NAME)

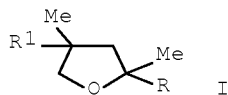


REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1986:115895 HCAPLUS Full-text
 DOCUMENT NUMBER: 104:115895
 ORIGINAL REFERENCE NO.: 104:18255a,18258a
 TITLE: Substituted tetrahydrofurans
 INVENTOR(S): Hochstetler, Alan R.
 PATENT ASSIGNEE(S): Givaudan Corp., USA
 SOURCE: U.S., 6 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 4549029	A	19851022	US 1983-482353	19830405
PRIORITY APPLN. INFO.:			US 1983-482353	19830405
OTHER SOURCE(S):	MARPAT	104:115895		

GI



AB Title compds. I [R = H, Me; R1 = optionally Me-substituted Ph, cyclohexenyl, cyclohexyl] were prepared and possess organoleptic properties described as fruity, citrus-like and reminiscent of grapefruit. I are useful in fragrances and flavors. Thus, 2,4-dimethyl-2-phenyl-4-pentenol was treated with LiAlH₄

to give 97% pentenol, which was cyclized with H₂SO₄ to give 77% I (R = Me, R₁ = Ph). The addition of 25 parts I to 975 parts citrus base having an odor characteristic of orange and lemon had a beneficial effect on the base, i.e., the citrus character was improved. I (R = Me, R₁ = 4-MeC₆H₄) provided the most desirable effect. The addition of 0.2 ppm I (R = Me, R₁ = Ph) to 100 g of a standard blueberry flavored drink enhanced the aroma and gave it a more natural blueberry flavor.

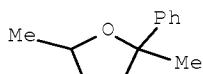
IT 100643-79-6P 100643-82-1P

RL: PREP (Preparation)

(preparation of, as flavoring and fragrance component)

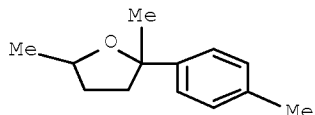
RN 100643-79-6 HCAPLUS

CN Furan, tetrahydro-2,5-dimethyl-2-phenyl- (CA INDEX NAME)



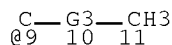
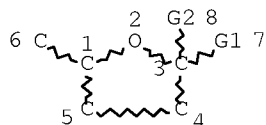
RN 100643-82-1 HCAPLUS

CN Furan, tetrahydro-2,5-dimethyl-2-(4-methylphenyl)- (CA INDEX NAME)



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L1 STR



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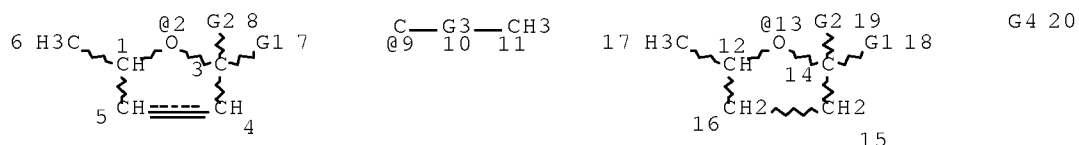
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NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

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VAR G2=N-BU/T-BU/S-BU/I-BU/9/CB

REP G3=(3-5) C

VAR G4=2/13

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

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L9 15 SEA FILE=HCAPLUS ABB=ON PLU=ON L5

L10 477297 SEA FILE=HCAPLUS ABB=ON PLU=ON ("ODOR AND ODOROUS SUBSTANCES"
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ION/CV OR ESSENCES/CV OR FLAVOR/CV) OR 320 OR ?FRAGR? OR
?ODOR? OR COSMETIC OR SHAMPOO OR DETERGEN? OR PERFUME OR
CLEANER OR LAUNDRY

L11 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 AND L10

L12 12 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 NOT L11

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L12 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:795177 HCAPLUS Full-text

DOCUMENT NUMBER: 149:152759

TITLE: Gold(I)-catalyzed cyclizations of 1,6-enynes:
alkoxycyclizations and exo/endo skeletal
rearrangements. [Erratum to document cited in
CA144:432480]

AUTHOR(S): Nieto-Oberhuber, Cristina; Munoz, M. Paz; Lopez,
Salome; Jemenez-Nunez, Eloisa; Nevado, Cristina;
Herrero-Gomez, Elena; Raducan, Mihai; Echavarren,
Antonio M.

CORPORATE SOURCE: Institute of Chemical Research of Catalonia (ICIQ),
Tarragona, 43007, Spain

SOURCE: Chemistry--A European Journal (2008), 14(17), 5096
CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors found that the configuration of diene 64 (Ar=p-MeOC₆H₄) in Scheme 6 on page 1683 was incorrectly assigned. The major isomer has a cis configuration, whereas the configuration of related compds. 62 and 66 (Ar=Ph and p-O₂NC₆H₄) is trans as reported. The correct version of the reaction is given.

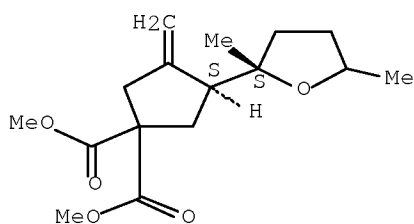
IT ~~884492-18-6P~~

RL: SPN (Synthetic preparation); PREP (Preparation)
(gold(I)-catalyzed cyclizations and exo/endo skeletal rearrangements of 1,6-enynes (Erratum))

RN 884492-18-6 HCAPLUS

CN 1,1-Cyclopentanedicarboxylic acid,
3-methylene-4-[(2R)-tetrahydro-2,5-dimethyl-2-furanyl]-, 1,1-dimethyl ester, (4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



L12 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:570848 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 147:174359

TITLE: Lewis acid character of zero-valent gold nanoclusters under aerobic conditions: intramolecular hydroalkoxylation of alkenes

AUTHOR(S): Kamiya, Ikuyo; Tsunoyama, Hironori; Tsukuda, Tatsuya; Sakurai, Hidehiro

CORPORATE SOURCE: Research Center for Molecular-Scale Nanoscience, Institute for Molecular Science, Myodaiji, Okazaki, 444-8787, Japan

SOURCE: Chemistry Letters (2007), 36(5), 646-647

CODEN: CMLTAG; ISSN: 0366-7022

PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:174359

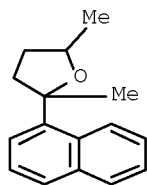
AB Gold nanoclusters stabilized by poly(N-vinyl-2-pyrrolidone) (Au:PVP NCs, ϕ = 1.3 nm) behave as Lewis acid catalyst in aqueous media under aerobic conditions, to promote the intramol. hydroalkoxylation of unactivated alkenes. Mol. oxygen generates a reaction center having the Lewis acidic character on the surface of Au NCs in which constituent gold atoms are formally in zero-valence state.

IT ~~1061284-19-2P~~

RL: SPN (Synthetic preparation); PREP (Preparation)
(Lewis acid character of zero-valent gold nanoclusters under aerobic conditions: intramol. hydroalkoxylation of alkenes)

RN 1061284-19-2 HCAPLUS

CN Furan, tetrahydro-2,5-dimethyl-2-(1-naphthalenyl)- (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:196741 HCAPLUS Full-text

DOCUMENT NUMBER: 144:432480

TITLE: Gold(I)-catalyzed cyclizations of 1,6-enynes: alkoxy cyclizations and exo/endo skeletal rearrangements

AUTHOR(S): Nieto-Oberhuber, Cristina; Munoz, M. Paz; Lopez, Salome; Jimenez-Nunez, Eloisa; Nevado, Cristina; Herrero-Gomez, Elena; Raducan, Mihai; Echavarren, Antonio M.

CORPORATE SOURCE: Institute of Chemical Research of Catalonia (ICIQ), Tarragona, 43007, Spain

SOURCE: Chemistry--A European Journal (2006), 12(6), 1677-1693
CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:432480

AB Gold(I) complexes are the most active catalysts for alkoxy- or hydroxycyclization and for skeletal rearrangement reactions of 1,6-enynes. Intramol. alkoxy cyclizations also proceed efficiently in the presence of gold(I) catalysts. Examples of the skeletal rearrangement of enynes by the endocyclic cyclization pathway are also documented. Iron(III) is also able to catalyze exo and endo skeletal rearrangements of 1,6-enynes, although the scope of this transformation is more limited. The gold(I)-catalyzed endocyclic cyclization proceeds by a mechanism different from those followed in the presence of PdII, HgII, or RhI catalysts.

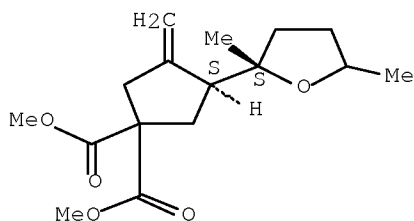
IT ~~884492-18-6P~~

RL: SPN (Synthetic preparation); PREP (Preparation)
(gold(I)-catalyzed cyclizations and exo/endo skeletal rearrangements of 1,6-enynes)

RN 884492-18-6 HCAPLUS

CN 1,1-Cyclopentanedicarboxylic acid,
3-methylene-4-[(2R)-tetrahydro-2,5-dimethyl-2-furanyl]-, 1,1-dimethyl ester, (4R)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 102 THERE ARE 102 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:511326 HCAPLUS Full-text
 DOCUMENT NUMBER: 143:172701
 TITLE: γ -Butyltelluro-2-butanol: a route to reactive 1,4-dianion intermediates
 AUTHOR(S): Princival, Jefferson L.; de Barros, Simone M. G.; Comasseto, Joao V.; Dos Santos, Alcindo A.
 CORPORATE SOURCE: DQF, Universidade Federal de Pernambuco, Recife, Pe, 50740-540, Brazil
 SOURCE: Tetrahedron Letters (2005), 46(26), 4423-4425
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 143:172701

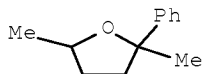
AB On reaction of γ -butyltelluro-2-butanol $\text{MeCH(OH)CH}_2\text{CH}_2\text{TeBu}$ with 2 equiv of n -butyllithium, both tellurium/lithium exchange and the proton abstraction reactions take place in a single step. The lithium dianion intermediate efficiently reacts with aldehydes and ketones R_1COR_2 [$\text{R}_1 = \text{Ph}$, 2-furyl, $\text{Me}_2\text{C:CHCH}_2\text{CH}_2\text{CHMeCH}_2$, $\text{R}_2 = \text{H}$; $\text{R}_1 = \text{Ph}$, $\text{R}_2 = \text{Me}$, Ph ; $\text{R}_1\text{R}_2 = (\text{CH}_2)_5$] producing the corresponding diols $\text{R}_1\text{R}_2\text{C(OH)CH}_2\text{CH}_2\text{CH(OH)Me}$ in 63-92% yields. The latter were readily converted into the corresponding 2-substituted-5-methyltetrahydrofurans by acid-catalyzed intramol. cyclodehydration.

IT 100643-79-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of unsym. 1,4-diols by addition of dianion, generated from γ -tellurobutanol, to aldehydes and ketones and their cyclodehydration to tetrahydrofurans)

RN 100643-79-6 HCAPLUS

CN Furan, tetrahydro-2,5-dimethyl-2-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:711234 HCAPLUS Full-text

DOCUMENT NUMBER: 141:379548
 TITLE: On the 6-endo Selectivity in 4-Penten-1-oxyl Radical Cyclizations
 AUTHOR(S): Hartung, Jens; Kneuer, Rainer; Rummey, Christian; Bringmann, Gerhard
 CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet Wuerzburg, Wuerzburg, D-97074, Germany
 SOURCE: Journal of the American Chemical Society (2004), 126(38), 12121-12129
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 141:379548

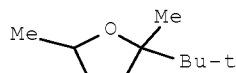
AB Regioselectivities in cyclizations of 4-substituted 4-penten-1-oxyl radicals were studied in a combined exptl. and computational study (d. functional theory). The progressive increase of the 6-endo-trig selectivity along 4-substituents $H < CH_3 < C(CH_3)_3 < C_6H_5$ were interpreted to originate from a balance between strain and FMO interactions. Torsional strain, which is associated with geometrical changes upon an approach of the reacting entities, is relevant for the 6-endo-trig but not for the 5-exo-trig reactions, as seen, for instance, in selective THF formation from the 4-penten-1-oxyl radical and its 4-Me derivative. The preference for tetrahydropyran formation in cyclizations of the 4-tert-Bu and the 4-phenyl-4-penten-1-oxyl radical was attributed to FMO interactions between the terminal carbon atom of the π bond and the O-radical center thus favoring the 6-endo-trig reaction from lower transition state energies.

IT 781665-93-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (6-endo selectivity in 4-penten-1-oxyl radical cyclizations)

RN 781665-93-8 HCAPLUS

CN Furan, 2-(1,1-dimethylethyl)tetrahydro-2,5-dimethyl- (CA INDEX NAME)



REFERENCE COUNT: 79 THERE ARE 79 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:651155 HCAPLUS Full-text

DOCUMENT NUMBER: 117:251155

ORIGINAL REFERENCE NO.: 117:43475a, 43478a

TITLE: Oxidative cyclization of 5-hydroxy alkenes with rhenium oxide, utilizing a co-oxidant. IV

AUTHOR(S): Tang, Suhan; Kennedy, Robert M.

CORPORATE SOURCE: Dep. Chem., Columbia Univ., New York, NY, 10027, USA

SOURCE: Tetrahedron Letters (1992), 33(37), 5303-6

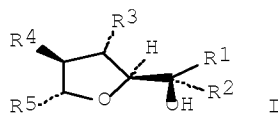
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:251155

GI



AB 5-Hydroxy alkenes, e.g., $R_1R_2C:CHCHR_3CHR_4CH(OH)R_5$ [$R_1 = (CH_2)_4Me$, $R_2 = R_3 = R_4 = R_5 = H$; $R_1 = R_3 = R_4 = R_5 = H$, $R_2 = (CH_2)_4Me$; $R_1 = R_4 = R_5 = H$, $R_2 = (CH_2)_5Me$, $R_3 = Me$; etc.], react with rhenium(VII) oxide in the presence of another oxidant, H_5IO_6 , to provide substituted tetrahydrofurans, e.g., I. The yield and stereoselectivity are comparable to stoichiometric results.

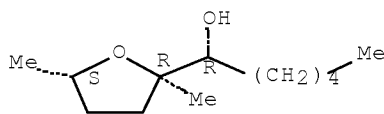
IT 143563-45-5P 144463-03-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 143563-45-5 HCAPLUS

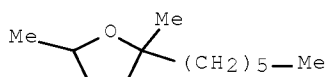
CN 2-Furanmethanol, tetrahydro-2,5-dimethyl- α -pentyl-,
[2 α (R*),5 β]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 144463-03-6 HCAPLUS

CN Furan, 2-hexyltetrahydro-2,5-dimethyl- (CA INDEX NAME)



L12 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:143739 HCAPLUS Full-text

DOCUMENT NUMBER: 114:143739

ORIGINAL REFERENCE NO.: 114:24405a

TITLE: Total synthesis of the meso-triterpene polyether
teurilene

AUTHOR(S): Hashimoto, Masaru; Harigaya, Hiroko; Yanagiya,
Mitsutoshi; Shirahama, Haruhisa

CORPORATE SOURCE: Fac. Sci., Hokkaido Univ., Sapporo, 060, Japan

SOURCE: Journal of Organic Chemistry (1991), 56(7), 2299-311

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:143739

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

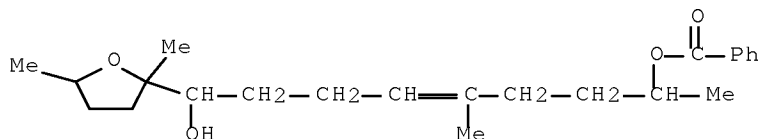
AB The first total synthesis of the triterpene ether teurilene (I) was accomplished utilizing two vanadium(V)-catalyzed oxidation-cyclization reactions with different stereoselectives. The synthesis involved stereoselective and step-by-step construction of 2,5-cis- and 2,5-trans-tetrahydrofuran rings, vanadium(V)-catalyzed oxidation of 4-substituted 4-en-1-ol II and subsequent cyclization of the resulting anti-epoxy alc. III, and a similar oxidation-cyclization of 5-substituted 4-en-1-ol IV by way of syn-epoxy alc. V. This was followed by construction of a third THF ring by more conventional means. An improved synthesis of I, which featured direct formation of a bis(tetrahydrofuran) from squalene derivative VI by simultaneous double oxidation-cyclization, was also accomplished.

IT 123908-75-8F

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 123908-75-8 HCAPLUS

CN 4-Nonene-1,8-diol, 5-methyl-1-(tetrahydro-2,5-dimethyl-2-furanyl)-,
8-benzoate, [2R-[2 α (1S*,4E,8S*),5 β]]- (9CI) (CA INDEX NAME)



L12 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:497852 HCAPLUS Full-text

DOCUMENT NUMBER: 113:97852

ORIGINAL REFERENCE NO.: 113:16541a,16544a

TITLE: Total syntheses of (+)-thyrsiferol, (+)-thyrsiferyl
23-acetate, and (+)-venustatriol

AUTHOR(S): Hashimoto, Masaru; Kan, Toshiyuki; Nozaki, Koji;
Yanagiya, Mitsutoshi; Shirahama, Haruhisa; Matsumoto,
Takeshi

CORPORATE SOURCE: Fac. Sci., Hokkaido Univ., Sapporo, 060, Japan

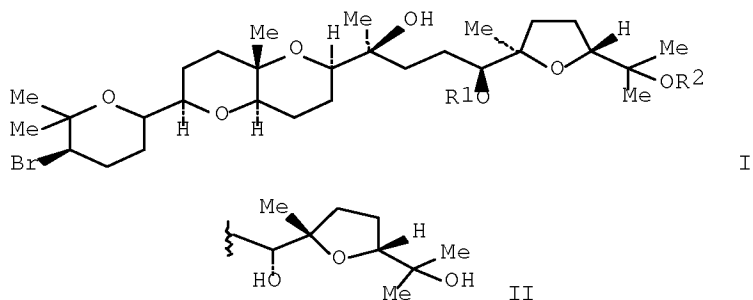
SOURCE: Journal of Organic Chemistry (1990), 55(17), 5088-107
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:97852

GI



AB The first total syntheses of (+)-thyrsiferol(I, R1 = R2 = H), (+)-thyrsiferyl 23-acetate (I, R1 = H, R2 = Ac), and (+)-venustatriol (II) were accomplished stereoselectively. An effective synthetic scheme to construct the BC ring system, which adopts a chair/twist-boat conformation, was first developed by means of a model study. This method involved stereoselective formation of the strained C ring by intramol. attack of the C7-hydroxyl group at the C3-position of the 2,3-epoxy alc., employing Ti(OCHMe2)4 as an acidic activator. Based on the information accumulated in the model study and retrosynthetic considerations, the total syntheses of the title compds. were performed in the sequence of (1) construction of the BC ring system equipped with a C1-C6 carbon unit, (2) elongation of the C17-C24 carbon chain, (3) formation of a D ring through the stereoselective epoxidn. of the 4-en-1-ol system and successive cyclization, and (4) construction of the A ring by bromonium ion induced cyclization of the 4-en-1-ol system.

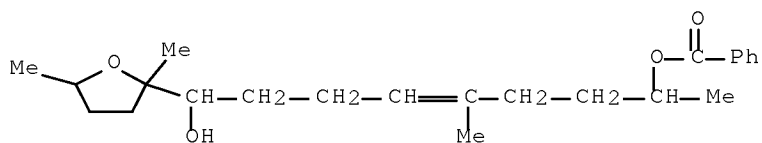
IT 123908-75-8P 128300-87-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and sequential mesylation and reaction with silver carbonate)

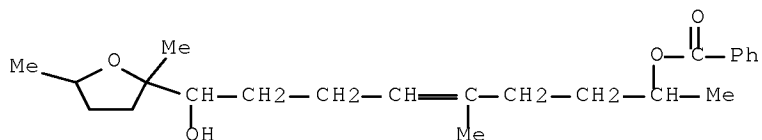
RN 123908-75-8 HCAPLUS

CN 4-Nonene-1,8-diol, 5-methyl-1-(tetrahydro-2,5-dimethyl-2-furanyl)-, 8-benzoate, [2R-[2 α (1S*,4E,8S*),5 β]]- (9CI) (CA INDEX NAME)



RN 128300-87-8 HCAPLUS

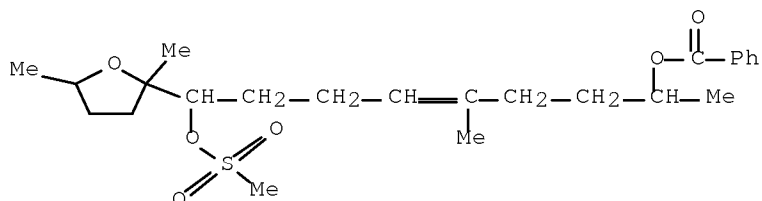
CN 4-Nonene-1,8-diol, 5-methyl-1-(tetrahydro-2,5-dimethyl-2-furanyl)-, 8-benzoate, [2S-[2 α (1S*,4E,8R*),5 α]]- (9CI) (CA INDEX NAME)



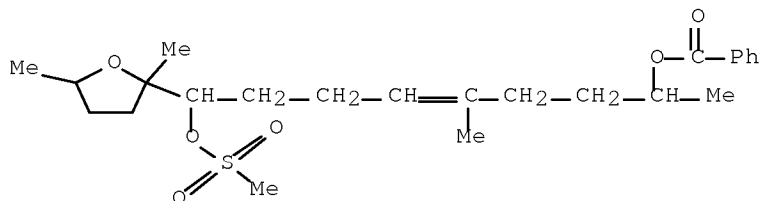
IT 128243-76-5P 128300-88-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 128243-76-5 HCAPLUS

CN 4-Nonene-1,8-diol, 5-methyl-1-(tetrahydro-2,5-dimethyl-2-furanyl)-,
8-benzoate 1-methanesulfonate, [2R-[2 α (1S*,4E,8S*),5 β]]- (9CI)
(CA INDEX NAME)

RN 128300-88-9 HCAPLUS

CN 4-Nonene-1,8-diol, 5-methyl-1-(tetrahydro-2,5-dimethyl-2-furanyl)-,
8-benzoate 1-methanesulfonate, [2S-[2 α (1S*,4E,8R*),5 α]]- (9CI)
(CA INDEX NAME)

L12 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:36220 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 112:36220

ORIGINAL REFERENCE NO.: 112:6277a,6280a

TITLE: Total synthesis of teurilene

AUTHOR(S): Hashimoto, Masaru; Harigaya, Hiroko; Yanagiya,
Mitsutoshi; Shirahama, Haruhisa

CORPORATE SOURCE: Fac. Sci., Hokkaido Univ., Sapporo, 060, Japan

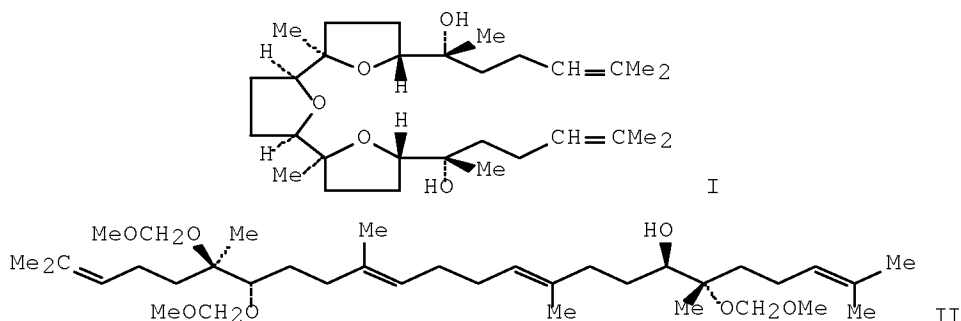
SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1988),
30, 119-25

CODEN: TYKYDS

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

GI



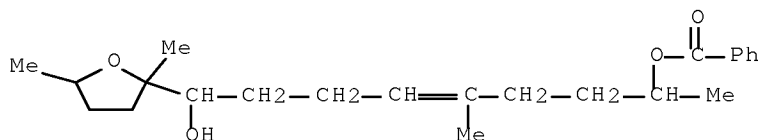
AB Teurilene (I), a marine triterpene isolated from red alga *Laurencia obtusa*, is characterized by an arrangement of eight asym. carbons in Cs symmetry,. The first total synthesis of I includes a short step synthesis by stereocontrolled double cyclization of a C30-squalene derivative (II).

IT 123908-75-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(epoxidn. of)

RN 123908-75-8 HCAPLUS

CN 4-Nonene-1,8-diol, 5-methyl-1-(tetrahydro-2,5-dimethyl-2-furanyl)-, 8-benzoate, [2R-[2 α (1S*,4E,8S*),5 β]]- (9CI) (CA INDEX NAME)



L12 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1980:514218 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 93:114218

ORIGINAL REFERENCE NO.: 93:18273a,18276a

TITLE: Synthesis of substituted tetrahydrofurans from γ -hydroxyketone tosylates

AUTHOR(S): Chastrette, Maurice; Axiotis, Georges P.

CORPORATE SOURCE: Lab. Chim. Org. Phys., Univ. Claude-Bernard, Villeurbanne, 69622, Fr.

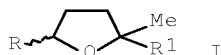
SOURCE: Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques (1980), 290(15), 305-7
CODEN: CHDCAQ; ISSN: 0567-6541

DOCUMENT TYPE: Journal

LANGUAGE: French

OTHER SOURCE(S): CASREACT 93:114218

GI



AB The reaction of p-MeC₆H₄SO₂OCHR(CH₂)₂COMe (R = H, Me) with organometallic reagents R₁M (M = MgBr, Li; R₁ = Bu, Ph, furyl) gave tetrahydrofurans I (same R, R₁).

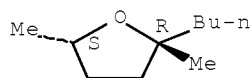
IT ~~74652-35-0P~~ ~~74652-36-1P~~ ~~74652-39-4P~~
~~74652-40-7P~~

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 74652-35-0 HCAPLUS

CN Furan, 2-butyltetrahydro-2,5-dimethyl-, cis- (9CI) (CA INDEX NAME)

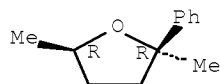
Relative stereochemistry.



RN 74652-36-1 HCAPLUS

CN Furan, tetrahydro-2,5-dimethyl-2-phenyl-, cis- (9CI) (CA INDEX NAME)

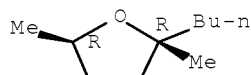
Relative stereochemistry.



RN 74652-39-4 HCAPLUS

CN Furan, 2-butyltetrahydro-2,5-dimethyl-, trans- (9CI) (CA INDEX NAME)

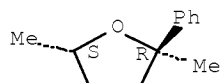
Relative stereochemistry.



RN 74652-40-7 HCAPLUS

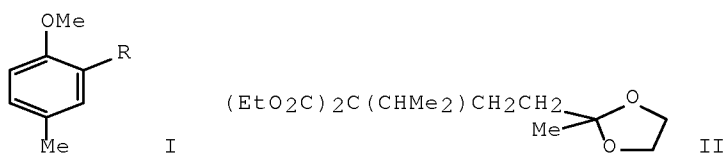
CN Furan, tetrahydro-2,5-dimethyl-2-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L12 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1980:146950 HCAPLUS Full-text

DOCUMENT NUMBER: 92:146950
 ORIGINAL REFERENCE NO.: 92:23893a,23896a
 TITLE: Syntheses of sesquichamenol methyl ether
 AUTHOR(S): Rohela, L. C.; Anand, R. C.
 CORPORATE SOURCE: Dep. Chem., Indian Inst. Technol., New Delhi, 110029, India
 SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1979), 17B(3), 207-10
 CODEN: IJSBDB; ISSN: 0376-4699
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



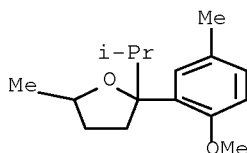
AB Sesquichamenol Me ether [I; R = CH(CHMe₂)CH₂CH₂COMe] was prepared either from ketal II by successive hydrolysis-decarboxylation, bromination-decarboxylation, ketal hydrolysis, and alkylation with I (R = Li), or by Wittig condensation of I (R = COCHMe₂) with MeOCH:PPh₃, hydrolysis of I [R = C(CHMe₂):CHOMe], condensation of I [R = CH(CHMe₂)CHO] with MeCOCH₂P(O)(OEt)₂, and hydrogenation of I [R = CH(CHMe₂)CH:CHCOMe].

IT 73256-90-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 73256-90-3 HCAPLUS

CN Furan, tetrahydro-2-(2-methoxy-5-methylphenyl)-5-methyl-2-(1-methylethyl)-
 (CA INDEX NAME)



L12 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1971:462786 HCAPLUS Full-text

DOCUMENT NUMBER: 75:62786

ORIGINAL REFERENCE NO.: 75:9951a,9954a

TITLE: Mechanism of photoenolization. o-Methylvalerophenone

AUTHOR(S): Bergmark, William R.; Beckmann, Brian; Lindenberger, William

CORPORATE SOURCE: Dep. Chem., Ithaca Coll., Ithaca, NY, USA

SOURCE: Tetrahedron Letters (1971), (25), 2259-62
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The photolysis of o-methylvalerophenone (I) gives o-MeC₆H₄COMe (II). The quantum yield of II is 0.010 vs. 0.41 quantum yield of PhCOMe from valerophenone. The yield-reducing effect of o-Me in I is due to photoenolization (i.e. the abstraction of 1 H from Me by the neighboring CO group). The contribution of photoelimination (i.e. the abstraction of γ -H) is small. The relative reactivities of Me and γ -H in I are .apprx.30:1. The decomposition of o-MeC₆H₄CBuMeOCl with uv light gave a mixture of chloro alcs., which after treatment with NaH in Et₂O gave 30.1 mixture of 1-butyl-1-methylisobenzofuran and o-(1,5-dimethyltetrahydrofuryl)toluene.

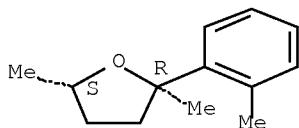
IT ~~33889-49-5P~~ ~~33889-50-8P~~

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 33889-49-5 HCAPLUS

CN Furan, tetrahydro-2,5-dimethyl-2-o-tolyl-, trans- (8CI) (CA INDEX NAME)

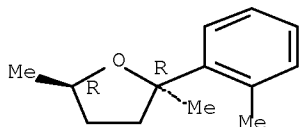
Relative stereochemistry.



RN 33889-50-8 HCAPLUS

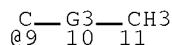
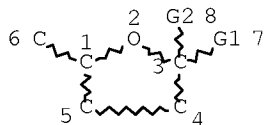
CN Furan, tetrahydro-2,5-dimethyl-2-o-tolyl-, cis- (8CI) (CA INDEX NAME)

Relative stereochemistry.



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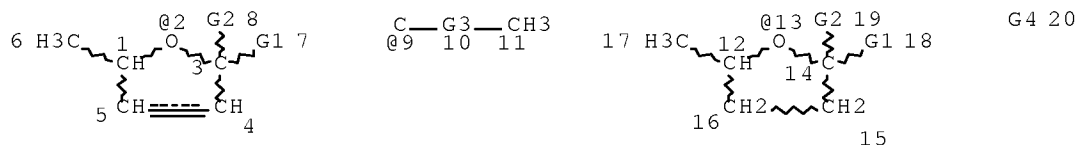
L1 STR



VAR G1=ME/ET/I-PR/N-PR
 VAR G2=N-BU/T-BU/S-BU/I-BU/9/CB
 REP G3=(3-5) C
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
 L3 1749 SEA FILE=REGISTRY SSS FUL L1
 L4 STR



VAR G1=ME/ET/I-PR/N-PR
 VAR G2=N-BU/T-BU/S-BU/I-BU/9/CB
 REP G3=(3-5) C
 VAR G4=2/13
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
 L5 28 SEA FILE=REGISTRY SUB=L3 SSS FUL L4
 L9 15 SEA FILE=HCAPLUS ABB=ON PLU=ON L5
 L10 477297 SEA FILE=HCAPLUS ABB=ON PLU=ON ("ODOR AND ODOROUS SUBSTANCES"
 /CV OR "ODOROUS SUBSTANCES"/CV OR ODORS/CV) OR ("AIR FRESHENERS
 "/CV OR "COSMETICS AND PERSONAL CARE PRODUCTS"/CV OR DEODORIZAT
 ION/CV OR ESSENCES/CV OR FLAVOR/CV) OR 320 OR ?FRAGR? OR
 ?ODOR? OR COSMETIC OR SHAMPOO OR DETERGEN? OR PERFUME OR
 CLEANER OR LAUNDRY
 L13 1721 SEA FILE=REGISTRY ABB=ON PLU=ON L3 NOT L5
 L14 1893 SEA FILE=HCAPLUS ABB=ON PLU=ON L13
 L15 9 SEA FILE=HCAPLUS ABB=ON PLU=ON L14(L) L10
 L16 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 NOT L9

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=> d ibib abs hitstr l16 1-8

L16 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2008:23427 HCAPLUS Full-text
 DOCUMENT NUMBER: 148:268924

TITLE: Cosmetic composition containing betula platyphylla extract and used for maintaining skin homeostasis
 INVENTOR(S): Lee, Jong Chan; Kim, Ji Hyeon; Kim, Yeon Jun; Baek, Seung Jae; Kim, Ji Yeong; Lee, Byeong Gon
 PATENT ASSIGNEE(S): Amorepacific Corp., S. Korea
 SOURCE: Repub. Korean Kongkae Taeho Kongbo, 8pp.
 CODEN: KRXXA7
 DOCUMENT TYPE: Patent
 LANGUAGE: Korean
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
KR 2007107254	A	20071107	KR 2006-39506	20060502
KR 869696	B1	20081121		

PRIORITY APPLN. INFO.: KR 2006-39506 20060502

AB The invention relates to the title cosmetic composition containing Betula platyphylla extract The composition can maintain the homeostasis of skin cell through normalizing the expression of the gene whose expression is reduced due to UV rays.

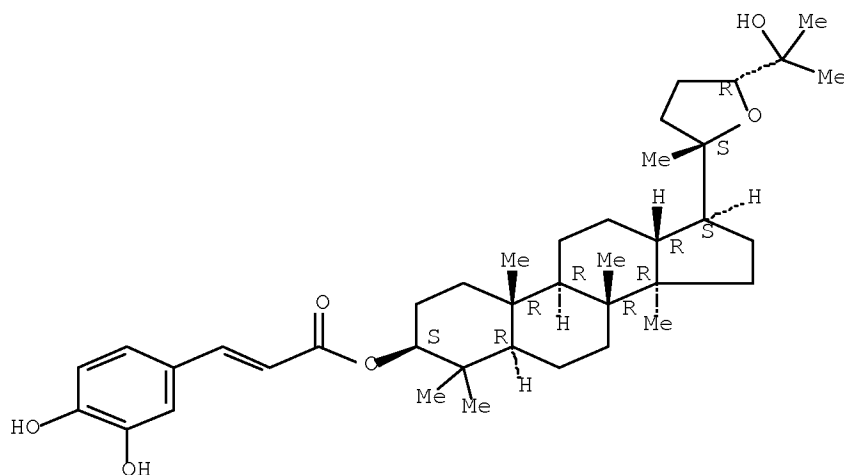
IT 1006710-67-3

RL: COS (Cosmetic use); NPO (Natural product occurrence); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
 (cosmetic composition containing betula platyphylla extract and used for maintaining skin homeostasis)

RN 1006710-67-3 HCAPLUS

CN Dammarane-3,25-diol, 20,24-epoxy-,
 3-[3-(3,4-dihydroxyphenyl)-2-propenoate], (3 β ,20S,24R)- (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



L16 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2007:391160 HCAPLUS Full-text

DOCUMENT NUMBER: 146:427828
 TITLE: Manufacture of antiaging cosmetic containing astragaloside IV
 INVENTOR(S): Zhang, Yindi; Yang, Yusong; Shen, Jianping; Zhao, Fuzhong; Zhuang, Binian; Sun, Shi; Zhang, Hanqing; Liu, Yuehui; You, Lifen
 PATENT ASSIGNEE(S): Nanjing Medical University, Peop. Rep. China
 SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 27pp.
 CODEN: CNXXEV
 DOCUMENT TYPE: Patent
 LANGUAGE: Chinese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1939254	A	20070404	CN 2006-10096725	20061012
PRIORITY APPLN. INFO.:			CN 2006-10096725	20061012

AB The cosmetic is composed of (by%): astragaloside IV (or total astragalosides) 0.0001-0.03 (0.0016-0.05), oil material and emulsifying agent 10-70, alkaline agent 0.2-2, humectant 5-21, antioxidant 0.0005-0.2, preservative 0.1-0.2, essence 0.5-1.5, and refined water 20-80. The cosmetic is manufactured by (1) heating oil material and emulsifying agent to 70-90, adding astragaloside IV, and stirring, (2) mixing alkaline agent, humectant, preservative and water according to the ratio, heating to 70-90 while stirring, maintaining for 20 min, and sterilizing, and (3) mixing the above solution, emulsifying while stirring, adding essence and antioxidant at 45-50, stirring, degassing, checking, and preparing into oil/water or water/oil skin-nursing frost.

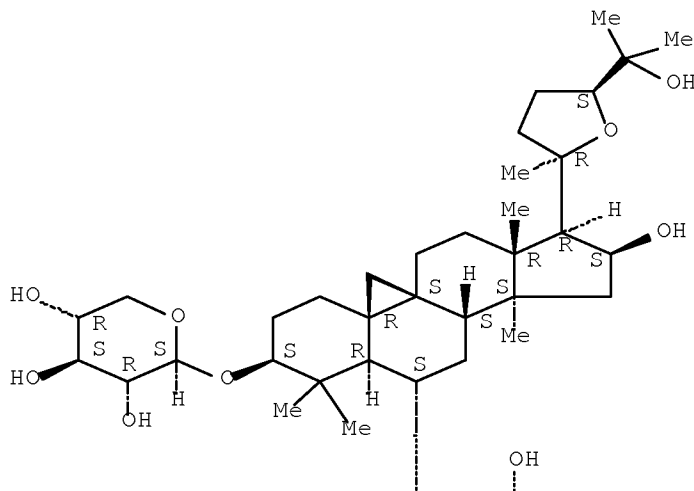
IT 84687-43-4, Astragaloside IV
 RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
 (manufacture of antiaging cosmetic containing astragaloside IV)

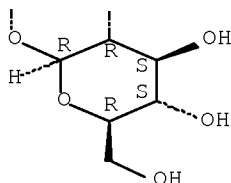
RN 84687-43-4 HCAPLUS

CN β -D-Glucopyranoside, (3 β , 6 α , 16 β , 20R, 24S)-20,24-epoxy-16,25-dihydroxy-3-(β -D-xylopyranosyloxy)-9,19-cyclolanostan-6-yl (CA INDEX NAME)

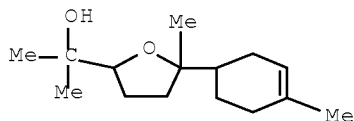
Absolute stereochemistry.

PAGE 1-A





L16 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2002:181935 HCAPLUS Full-text
 DOCUMENT NUMBER: 137:231533
 TITLE: New developments in sorptive extraction for the analysis of flavours and fragrances
 AUTHOR(S): Sandra, P.; David, F.; Vercammen, J.
 CORPORATE SOURCE: Department of Organic Chemistry, University of Gent, Ghent, 9000, Belg.
 SOURCE: Special Publication - Royal Society of Chemistry (2002), 277(Advances in Flavours and Fragrances), 27-38
 CODEN: SROCD0; ISSN: 0260-6291
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The principle was presented of stir bar sorptive extraction (SBSE) and head space sorptive extraction (HSSE). Applicability was illustrated of SBSE- and HSSE-capillary gas chromatog./mass spectrometry with the anal. of flavor carriers in tea, beer, yogurt, and bananas, off-flavors in beer, and bitter compds. in beer.
 IT ~~55399-12-7~~, Bisabolol oxide B
 RL: ANT (Analyte); ANST (Analytical study)
 (sorptive extraction for the anal. of flavors and fragrances)
 RN 55399-12-7 HCAPLUS
 CN 2-Furanmethanol, tetrahydro- $\alpha,\alpha,5$ -trimethyl-5-(4-methyl-3-cyclohexen-1-yl)- (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2000:713757 HCAPLUS Full-text
 DOCUMENT NUMBER: 133:325438
 TITLE: Supercritical extraction of chamomile for use in

cosmetics
 AUTHOR(S): Simandi, Bela; Sawinsky, Janos; Deak, Andras; Domokos, Janos; Hethelyi, Eva; Palinkas, Janos
 CORPORATE SOURCE: Hung.
 SOURCE: Olaj, Szappan, Kozmetika (2000), 49(Kulonszam), 48-52
 CODEN: OSZKAT; ISSN: 0472-8602
 PUBLISHER: METE
 DOCUMENT TYPE: Journal
 LANGUAGE: Hungarian

AB Chamomile was extracted by supercrit. fluid extraction (SFE) and for comparison, with two solvents: ethanol and hexane. The SFE process was optimized by the variation of the temperature and pressure applied. Volatile components, oils were determined by GC. The SFE extract and the ethanol extract were used in cream and body lotion formulations and their properties were compared. The SFE extract had a richer chamomile aroma than the ethanol extract, according to the organoleptic test. Skin moisturizing effects were measured using a

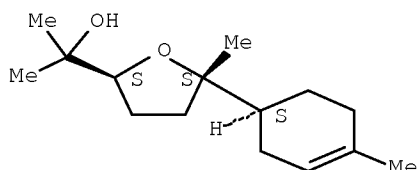
CM 80 corneometer; there were no statistically significant differences between the two exts. Transepidermal water loss was evaluated with an evaporimeter; the SFE exts. were faster in restoring the normal skin barrier function. This is due probably to the fact that the SFE ext. contains more waxy components. The two exts. in the cosmetic prepn. had the same effects on skin pH and lipid content.

IT 26184-88-3P, Bisabolol oxide II
 RL: ANT (Analyte); BOC (Biological occurrence); BSU (Biological study, unclassified); PUR (Purification or recovery); ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
 (supercrit. extraction of chamomile for use in cosmetics)

RN 26184-88-3 HCAPLUS

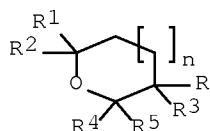
CN 2-Furanmethanol, tetrahydro- $\alpha,\alpha,5$ -trimethyl-5-[(1S)-4-methyl-3-cyclohexen-1-yl]-, (2S,5S)- (CA INDEX NAME)

Absolute stereochemistry.

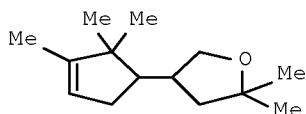


L16 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1996:314050 HCAPLUS Full-text
 DOCUMENT NUMBER: 125:86473
 ORIGINAL REFERENCE NO.: 125:16301a,16304a
 TITLE: Preparation of cycloalkyltetrahydrofurans and analogs as perfume fragrances
 INVENTOR(S): Noire, Paul D.
 PATENT ASSIGNEE(S): Givaudan-Roure Corporation, USA
 SOURCE: U.S., 31 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5510326	A	19960423	US 1994-363685	19941223
WO 9620185	A2	19960704	WO 1995-EP5002	19951218
WO 9620185	A3	19960906		
W: JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 746552	A1	19961211	EP 1995-942177	19951218
EP 746552	B1	20020612		
R: CH, DE, ES, FR, GB, IT, LI, NL				
JP 11505511	T	19990521	JP 1995-520178	19951218
ES 2176353	T3	20021201	ES 1995-942177	19951218
US 5665696	A	19970909	US 1995-577487	19951222
PRIORITY APPLN. INFO.:			US 1994-363685	A 19941223
			WO 1995-EP5002	W 19951218
OTHER SOURCE(S):		MARPAT 125:86473		
GI				



I



II

AB Title compds. [e.g., I; R = (cyclo)alkyl; R1 = alkyl; R2 = H or alkyl; R3 = H or Me; n = 0 and R4 = R5 = H; n = 1 and R4, R5 = H or alkyl] were prepared. Thus, 2,2,3-trimethyl-3-cyclopenteneacetaldehyde was alkylated by CH₂:CMeCH₂OH and the reduced product cyclized to give title compound II of woody amber fragrance.

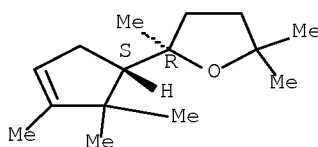
IT 178744-79-1P 178744-80-4P

RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of cycloalkyltetrahydrofurans and analogs as perfume fragrances)

RN 178744-79-1 HCAPLUS

CN Furan, tetrahydro-2,2,5-trimethyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-, (R*, S*)- (9CI) (CA INDEX NAME)

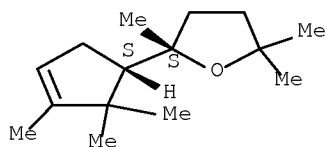
Relative stereochemistry.



RN 178744-80-4 HCAPLUS

CN Furan, tetrahydro-2,2,5-trimethyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-, (R*, R*)- (9CI) (CA INDEX NAME)

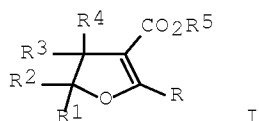
Relative stereochemistry.



L16 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1989:23713 HCAPLUS Full-text
 DOCUMENT NUMBER: 110:23713
 ORIGINAL REFERENCE NO.: 110:4005a,4008a
 TITLE: Preparation of 4-alkoxycarbonyl-2,3-dihydrofurans as
 aroma enhancers
 INVENTOR(S): Harris, Eugene C.; Fayter, Richard C., Jr.
 PATENT ASSIGNEE(S): National Distillers and Chemical Corp., USA
 SOURCE: U.S., 12 pp. Cont.-in-part of 4,636,571.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4681703	A	19870721	US 1986-870594	19860604
US 4515978	A	19850507	US 1983-503974	19830613
US 4636571	A	19870113	US 1985-726220	19850423
PRIORITY APPLN. INFO.:			US 1983-503974	A2 19830613
			US 1985-726220	A2 19850423

GI

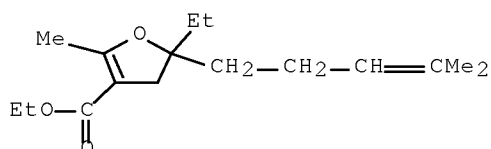


AB Title compds. I (R = C1-5 alkyl; R1, R5 = C1-4 alkyl; R2 = H, C1-6 alkyl; R3, R4 = H, Me), useful as fragrance compns. that can also be used in conjunction with known fragrance materials to enhance or augment the aroma itself, were prepared either by isomerization of the corresponding cyclopropyl ketone derivs. or from oxidative 1,2-addition of 1,3-dicarbonyl compds. to conjugated dienes in AcOH containing Mn and a catalytic amount of Cu. I (R3 = R4 = H) are also prepared by condensation of R1R2CHCHO with RCOCH2CO2R5 followed by cyclization. Thus, reaction of Me2CHCHO and AcCH2CO2Et in the presence of a small amount of piperidine gave Me2CHCH:C(Ac)CO2Et which was refluxed 2 h in PhMe containing Ac2O and 4-MeC6H4SO2OH to give I (R-R2 = Me, R3 = R4 = H, R5 = Et) which had a chamomile and jasmine character.

IT 109176-06-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, for fragrance compns.)

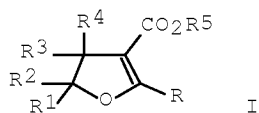
RN 109176-06-9 HCAPLUS
 CN 3-Furancarboxylic acid, 5-ethyl-4,5-dihydro-2-methyl-5-(4-methyl-3-penten-1-yl)-, ethyl ester (CA INDEX NAME)



L16 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1987:439592 HCAPLUS Full-text
 DOCUMENT NUMBER: 107:39592
 ORIGINAL REFERENCE NO.: 107:6615a,6618a
 TITLE: 4-Carbalkoxy-2-ethyl-2,3-dihydrofurans for fragrance compositions
 INVENTOR(S): Harris, Eugene G.; Fayter, Richard G., Jr.
 PATENT ASSIGNEE(S): National Distillers and Chemical Corp., USA
 SOURCE: U.S., 11 pp. Cont.-in-part of U.S. 4,515,978.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

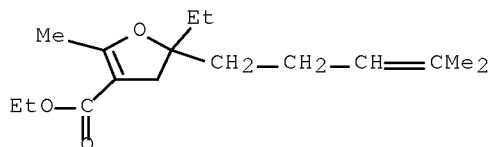
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4636571	A	19870113	US 1985-726220	19850423
US 4515978	A	19850507	US 1983-503974	19830613
US 4681703	A	19870721	US 1986-870594	19860604
PRIORITY APPLN. INFO.:			US 1983-503974	A2 19830613
			US 1985-726220	A2 19850423

GI



AB Title compds. I (R = C1-5 alkyl; R1, R5 = C1-4 alkyl; R2 = H, C1-6 alkyl; R3, R4 = H, Me), useful as fragrance compns. that can also be used in conjunction with known fragrance materials to enhance or augment the aroma itself, were prepared I are prepared either by isomerization of the corresponding cyclopropyl ketone derivs. or from oxidative 1,2-addition of 1,3-dicarbonyl compds. to conjugated dienes in AcOH containing Mn and a catalytic amount of Cu. Oxidative addition of MeCOCH2CO2Et to H2C:CHCH:CH2 in presence of Mn(OAc)2, AcOH and Cu(OAc)2 gave 4-carbethoxy-5-methyl-2-vinyl-2,3-dihydrofuran, which was hydrogenated to give I (R = Me; R1, R3, R4 = H; R2, R5 = Et) which when added to a common herbal perfume base at 1 weight% imparted a desirable chamomile nuance to the overall odor character.

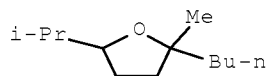
IT 109176-06-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, for fragrance compns.)
 RN 109176-06-9 HCAPLUS
 CN 3-Furancarboxylic acid, 5-ethyl-4,5-dihydro-2-methyl-5-(4-methyl-3-penten-1-yl)-, ethyl ester (CA INDEX NAME)



L16 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1985:437327 HCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 103:37327
 ORIGINAL REFERENCE NO.: 103:6051a,6054a
 TITLE: Search for new aroma chemicals: cyclic ethers from methyl heptenone
 AUTHOR(S): Mohindru, R. N.; Koul, S. K.; Sethi, V. K.; Taneja, S. C.; Dhar, K. L.
 CORPORATE SOURCE: Reg. Res. Lab., Jammu Tawi, 180001, India
 SOURCE: PAFAI Journal (1984), 6(3), 15-18
 CODEN: PAFJDI; ISSN: 0255-7177
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

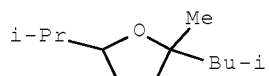


AB Grignard reaction of the readily available synthon $\text{Me}_2\text{C}:\text{CH}(\text{CH}_2)_2\text{COMe}$ with RX (R = C1-6 alkyl, Ph, aralkyl, X = halo) gave $\text{Me}_2\text{C}:\text{CH}(\text{CH}_2)_2\text{CRMMeOH}$ (I), oxymercuration-demercuration of which gave mixts. of tetrahydrofurans II and tetrahydropyrans III. I-III were evaluated as aroma compds. for perfumery.
 IT 97265-03-7P 97265-04-8P 97265-05-9P
 97265-06-0P 97265-07-1P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and odor of)
 RN 97265-03-7 HCAPLUS
 CN Furan, 2-butyltetrahydro-2-methyl-5-(1-methylethyl)- (CA INDEX NAME)



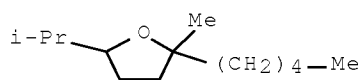
RN 97265-04-8 HCAPLUS

CN Furan, tetrahydro-2-methyl-5-(1-methylethyl)-2-(2-methylpropyl)- (CA INDEX NAME)



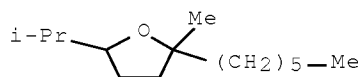
RN 97265-05-9 HCAPLUS

CN Furan, tetrahydro-2-methyl-5-(1-methylethyl)-2-pentyl- (CA INDEX NAME)



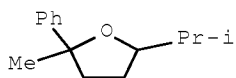
RN 97265-06-0 HCAPLUS

CN Furan, 2-hexyltetrahydro-2-methyl-5-(1-methylethyl)- (CA INDEX NAME)



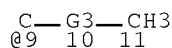
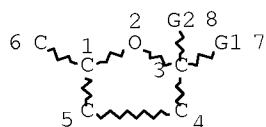
RN 97265-07-1 HCAPLUS

CN Furan, tetrahydro-2-methyl-5-(1-methylethyl)-2-phenyl- (CA INDEX NAME)



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L1 STR



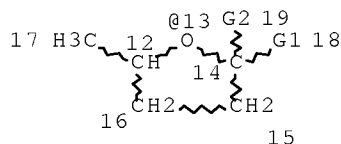
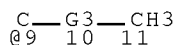
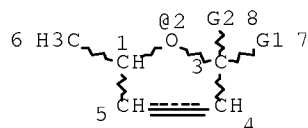
VAR G1=ME/ET/I-PR/N-PR
 VAR G2=N-BU/T-BU/S-BU/I-BU/9/CB
 REP G3=(3-5) C
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

L3 1749 SEA FILE=REGISTRY SSS FUL L1

L4 STR



G4 20

VAR G1=ME/ET/I-PR/N-PR
 VAR G2=N-BU/T-BU/S-BU/I-BU/9/CB
 REP G3=(3-5) C
 VAR G4=2/13
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L5 28 SEA FILE=REGISTRY SUB=L3 SSS FUL L4

L9 15 SEA FILE=HCAPLUS ABB=ON PLU=ON L5

L10 477297 SEA FILE=HCAPLUS ABB=ON PLU=ON ("ODOR AND ODOROUS SUBSTANCES"
 /CV OR "ODOROUS SUBSTANCES"/CV OR ODORS/CV) OR ("AIR FRESHENERS"
 /CV OR "COSMETICS AND PERSONAL CARE PRODUCTS"/CV OR DEODORIZAT
 ION/CV OR ESSENCES/CV OR FLAVOR/CV) OR 320 OR ?FRAGR? OR
 ?ODOR? OR COSMETIC OR SHAMPOO OR DETERGEN? OR PERFUME OR
 CLEANER OR LAUNDRY

L11 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 AND L10

L12 12 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 NOT L11

L13 1721 SEA FILE=REGISTRY ABB=ON PLU=ON L3 NOT L5
 L14 1893 SEA FILE=HCAPLUS ABB=ON PLU=ON L13
 L37 94 SEA FILE=HCAPLUS ABB=ON PLU=ON KRAFT PHILIP ?/AU OR KRAFT
 P/AU OR KRAFT P ?/AU OR KRAFT PHILIP/AU
 L38 0 SEA FILE=HCAPLUS ABB=ON PLU=ON L37 AND L14
 L43 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L37 AND ?FURAN?
 L44 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L43 NOT (L11 OR L12)
 L45 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L38 OR L44

=> d ibib abs hitstr l45 1-6

L45 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2008:1480900 HCAPLUS Full-text
 TITLE: 2,5-DI- AND 2,2,5-TRISUBSTITUTED DI- AND
 TETRAHYDROFURAN DERIVATIVES AND THEIR USE FOR THE
 PRODUCTION OF PERFUMES
 INVENTOR(S): Kraft, Philip
 PATENT ASSIGNEE(S): Givaudan SA, Switz.
 SOURCE: PCT Int. Appl., 19pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008148236	A1	20081211	WO 2008-CH249	20080603
W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.: GB 2007-10700 A 20070605
 AB Di-/trisubstituted furans of the formula (I) and their use as odorants wherein
 R1 is hydrogen or methyl; R2 is Et, Pr or isopropyl; the bond between C-3 and
 C-4 is a single bond, or the dotted line together with the bond between C-3
 and C-4 represents a double bond; and the bond between C-4' and C-5' is a
 single bond, or the dotted line together with the bond between C-4' and C-5'
 represents a double bond, either in (E)- or (Z)- configuration. The
 invention furthermore relates to a method of their production and to perfume
 compns. comprising them.
 REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2008:490315 HCAPLUS Full-text
 DOCUMENT NUMBER: 149:86911
 TITLE: Unexpected tethering in the synthesis of
 methyl-substituted acetyl-1-oxaspiro[4.5]decanes:

novel Woody-Ambery odorants with improved bioavailability

AUTHOR(S): Kraft, Philip; Popaj, Kasim

CORPORATE SOURCE: Givaudan Schweiz AG, Fragrance Research, Duebendorf, Switz.

SOURCE: European Journal of Organic Chemistry (2008), (2), 261-268
CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB To study the olfactory properties of spirocyclic analogs of an Iso Gamma with improved water solubility and bioavailability, it was envisaged to spiroannulate 1-acetyl-1,2-dimethylcyclohexanone at the 4-position with a 3,3-dimethyltetrahydrofuran-2-yl moiety that would mimic the polarity of the double bond by its ether function. 3,3-Dimethyl-4-methylenehex-5-en-1-ol was prepared by copper(I)-mediated 1,4-conjugate addition of the Grignard reagent of chloroprene to 3-methylbut-2-enal with subsequent LAH reduction. However, the Diels-Alder reaction of the diene with (E)-3-methylpent-3-en-2-one in the presence of Me₂AlCl unexpectedly provided exclusively the undesired meta adduct, as was discovered after cyclization to 11 with MeSO₃H. The wrong selectivity was due to a tethering effect of the Lewis acid, and this could be evaded by changing the carbonyl function of the dienophile to a hydroxy group. Thereby the (5'R*, 7'S*, 8'S*)-configured 1-(4',4',7',8'-tetramethyl-1'-oxaspiro[4.5]decan-7'/8'-yl)ethan-1-ones, as well as the like-configured 1-(4',4',7'-trimethyl-1'-oxaspiro[4.5]-decan-7'/8'-yl)ethan-1-ones, were prepared selectively and studied for their odor characters, threshold values, and octanol/water partition coeffs.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1215756 HCAPLUS Full-text

DOCUMENT NUMBER: 143:465642

TITLE: Preparation of alicyclic carboxylic acid oxycarbonylmethyl esters and their use as odorants

INVENTOR(S): Kraft, Philip

PATENT ASSIGNEE(S): Givaudan S. A., Switz.

SOURCE: PCT Int. Appl., 16 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

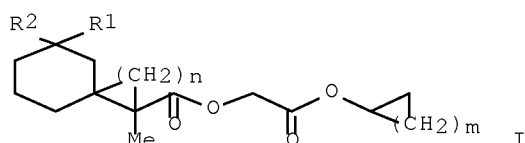
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005108534	A1	20051117	WO 2005-CH251	20050504
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,			

RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG

EP 1743013	A1	20070117	EP 2005-732413	20050504
EP 1743013	B1	20071219		
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1950490	A	20070418	CN 2005-80014642	20050504
BR 2005009666	A	20071009	BR 2005-9666	20050504
JP 2007536285	T	20071213	JP 2007-511828	20050504
AT 381605	T	20080115	AT 2005-732413	20050504
ES 2297694	T3	20080501	ES 2005-732413	20050504
US 20070225201	A1	20070927	US 2006-568475	20061030
MX 2006PA12767	A	20070116	MX 2006-PA12767	20061103
KR 2007006895	A	20070111	KR 2006-723223	20061106
IN 2006CN04090	A	20070629	IN 2006-CN4090	20061107
PRIORITY APPLN. INFO.:			GB 2004-10134	A 20040507
			WO 2005-CH251	W 20050504

GI



AB Alicyclic carboxylic acid oxycarbonylmethyl esters (I; R1, R2 = H, Me; n = 0, 1; m = 0, 1) were prepared for use as odorants. Thus, a perfume was prepared containing bergamot oil 40, p-tert-Butylcyclohexyl acetate 150, citral 5, γ -decalactone 4, p-cresyl Me ether 5, 4,5-dimethyl-3-hydroxy-2(5H)-furanone @ 1 % in tri-Et citrate 2, dodecanal 2, guaiyl acetate 10, (3Z)-hex-3-enol @ 10 % in dipropylene glycol 4, hexyl acetate 50, β -ionone 40, linalool 20, linalyl acetate 13, Me dihydrojasmonate 100, nonayl acetate 50, 3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-4-penten-2-ol 1, octahydrocoumarin 10, phenoxyethyl alc. 140, 2-phenylethyl acetate 12, 2-phenylethyl alc. 80, sweet orange oil 50, 3a,6,6,9a-tetramethyldodecahydronaphtho[2,1-b]furan 2 (6E)-3,7,11-trimethyl-6,10-dodecadienal 30, 1,7,7-trimethyl-2'-(isopropyl)spiro-[bicyclo[2.2.1]heptane-2,4'-[1,3]dioxane] @ 50 % in iso-Pr myristate 30, and 2-(3,3-dimethylcyclohexyl)propionic acid ethoxycarbonylmethyl ester (preparation given) 150 parts, resp.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:1120781 HCAPLUS Full-text

DOCUMENT NUMBER: 142:197812

TITLE: On the scope of a Prins-type cyclization of oxonium ions

AUTHOR(S): Frater, Georg; Mueller, Urs; Kraft, Philip

CORPORATE SOURCE: Givaudan Schweiz AG, Fragrance Research, Duebendorf, CH-8600, Switz.

SOURCE: Helvetica Chimica Acta (2004), 87(11), 2750-2763

CODEN: HCACAV; ISSN: 0018-019X

PUBLISHER: Verlag Helvetica Chimica Acta

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:197812

AB The Prins cyclization of an aldehyde with a homoallylic alc., affording tetrahydro-2H-pyrans via the oxonium ion as central intermediate, was conceptually transferred to (alk-3-enyloxy)acrylates, which form a related oxonium ion upon treatment with acids. The scope and utility of this modification of the Prins-type cyclization of oxonium ions is discussed exemplarily by means of the syntheses of ten tetrahydro-2H-pyran and THF derivs., featuring diverse substitution patterns as well as different degrees of mol. complexity. These target structures include (±)-Et (2RS)-2-[(2RS,4SR,6RS)- and (2SR,4RS,6SR)-2-tetrahydro-4-hydroxy-6-methylpyran-2-yl]propanoate, (±)-Et [(2RS,3RS)-tetrahydro-3-isopropenylfuran-2-yl]acetate, (±)-Et (2Z)-3-(tetrahydro-2,2-dimethylfuran-3-yl)acrylate, (±)-(3aRS,6RS,7aRS)-octahydro-7a-methylbenzofuran-6-yl formate, (±)-Et (2RS,3RS,4aRS,8SR,8aRS)-hexahydro-2,5,5,8-tetramethyl-7-oxo-2H,5H-pyrano[4,3-b]pyran-3-carboxylate, and (±)-Et (2RS,3RS,6SR)-tetrahydro-6-(2-methoxy-2-oxoethyl)-3-methyl-2H-pyran-2-carboxylate. Besides the stereochem. and mechanistic details of this versatile oxonium-ion cyclization, the synthesis of suitable starting materials is also described.

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L45 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:25885 HCAPLUS Full-text

DOCUMENT NUMBER: 126:74626

ORIGINAL REFERENCE NO.: 126:14441a,14444a

TITLE: Our tactics in ring enlargement. Construction of medium and large ring compounds

AUTHOR(S): Tochtermann, Werner; Kraft, Philip

CORPORATE SOURCE: Inst. Org. Chem., Univ. Kiel, Kiel, D-24098, Germany

SOURCE: Synlett (1996), (11), 1029-1035
CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER: Thieme

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with 59 refs. on the authors tactics in the synthesis of medium and large ring compds. First the application of an oxanorbornadiene-oxepine ring enlargement to the synthesis of a [6]paracyclophane, of hydroazulenes, and bridged furanoses is described. Transformations of the Diels-Alder adduct of cyclooctyne and furan led to the synthesis of (-)-muricatacin and guided the way into fragrance chemical. Finally the stereoselective synthesis of macrocyclic odorants by way of ring enlargement of cycloalkanones with chiral building blocks is highlighted.

L45 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:700497 HCAPLUS Full-text

DOCUMENT NUMBER: 121:300497

ORIGINAL REFERENCE NO.: 121:55001a,55004a

TITLE: Synthesis of medium and large ring compounds. XXXVII. Synthesis and olfactory properties of (Z)-5,6-dimethylcyclododec-5-en-1-one and (Z)-(±)-5,6-dimethylcyclododec-5-en-1-ol

AUTHOR(S): Kraft, Philip; Tochtermann, Werner

CORPORATE SOURCE: Inst. fuer Organische Chem., Universitaet Kiel, Kiel, D-24098, Germany

SOURCE: Liebigs Annalen der Chemie (1994), (8), 827-30
CODEN: LACHDL; ISSN: 0170-2041

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:300497

AB According to mol. modeling calcns. the title compound 13 should fit the olfactory receptor of trans-10-ethyltetrahydroionol (1). In order to check this prediction the target mol. 13 and ketone 12 have been synthesized by starting from cyclooctyne and ~~furan~~. Cleavage of the oxanorbornene bridge of the selectively hydrogenated Diels-Alder adduct 5 with LTBAH/triethylborane, oxidation, epoxidn. and α,β -epoxyketone \rightarrow alkynone fragmentation result in a ring enlargement of cyclooctyne by an oxotetramethylene unit. Key reaction is the diboration of cycloalkynone 9 followed by a Suzuki coupling with iodomethane. Reduction of ketone 12 gives the desired dimethylcyclododecenol 13, which possesses only a weak cedarwood note. In contrast, the corresponding ketone 12 has an intensive odor described as dry, cedarwood-like with interesting cooling animal facets.

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(FILE 'HOME' ENTERED AT 11:48:08 ON 24 DEC 2008)

FILE 'REGISTRY' ENTERED AT 11:48:17 ON 24 DEC 2008

L1 STR
L3 1749 SEA SSS FUL L1
L4 STR
L5 28 SEA SUB=L3 SSS FUL L4

FILE 'HCAPLUS' ENTERED AT 11:55:55 ON 24 DEC 2008

L9 15 SEA ABB=ON PLU=ON L5
L10 477297 SEA ABB=ON PLU=ON ("ODOR AND ODOROUS SUBSTANCES"/CV OR
"ODOROUS SUBSTANCES"/CV OR ODORS/CV) OR ("AIR FRESHENERS"/CV
OR "COSMETICS AND PERSONAL CARE PRODUCTS"/CV OR DEODORIZATION/C
V OR ESSENCES/CV OR FLAVOR/CV) OR 320 OR ?FRAGR? OR ?ODOR? OR
COSMETIC OR SHAMPOO OR DETERGEN? OR PERFUME OR CLEANER OR
LAUNDRY
L11 3 SEA ABB=ON PLU=ON L9 AND L10
D STAT QUE L11
D IBIB ABS HITSTR L11 1-3
L12 12 SEA ABB=ON PLU=ON L9 NOT L11
D STAT QUE L12
D IBIB ABS HITSTR L12 1-12

FILE 'REGISTRY' ENTERED AT 11:58:41 ON 24 DEC 2008

L13 1721 SEA ABB=ON PLU=ON L3 NOT L5

FILE 'HCAPLUS' ENTERED AT 11:59:07 ON 24 DEC 2008

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L37 94 SEA ABB=ON PLU=ON KRAFT PHILIP ?/AU OR KRAFT P/AU OR KRAFT P
?/AU OR KRAFT PHILIP/AU
L38 0 SEA ABB=ON PLU=ON L37 AND L14
L43 8 SEA ABB=ON PLU=ON L37 AND ?FURAN?
L44 6 SEA ABB=ON PLU=ON L43 NOT (L11 OR L12)
L45 6 SEA ABB=ON PLU=ON L38 OR L44
D STAT QUE L45
D IBIB ABS HITSTR L45 1-6

FILE HOME

FILE REGISTRY

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FILE LAST UPDATED: 23 Dec 2008 (20081223/ED)

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